Flagellum Pumping Efficiency in Shear-Thinning Viscoelastic Fluids – Supplementary Material

1 Non-Dimensionalization of Equations

The coupled equations of motion are

$$\rho \frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} = \mu_{\mathrm{n}} \Delta \mathbf{u}(\mathbf{x},t) - \nabla p(\mathbf{x},t) + \frac{\mu_{\mathrm{p}}}{\lambda} \nabla \cdot \mathbb{C}(\mathbf{x},t) + \mathbf{f}(\mathbf{x},t), \tag{1}$$

$$\overset{\triangledown}{\mathbb{C}}(\mathbf{x},t) = -\frac{1}{\lambda}(\mathbb{C}(\mathbf{x},t) - \mathbb{I}) - \frac{\alpha}{\lambda}(\mathbb{C}(\mathbf{x},t) - \mathbb{I})^2, \tag{2}$$

$$\nabla \cdot \mathbf{u}(\mathbf{x},t) = 0, \tag{3}$$

in which $\mathbf{u}(\mathbf{x},t)$ is the fluid velocity, $\mathbb{C}(\mathbf{x},t)$ is the conformation tensor associated with the Giesekus fluid, $p(\mathbf{x},t)$ is the pressure, ρ the density, μ_{n} the viscosity of the solvent, μ_{p} the polymer viscosity, λ is the characteristic stress relaxation time associated with the fluid, and α is the Giesekus nonlinearity parameter that controls the degree of nonlinear dependence of the shear stress on shear rate.[1] The force density $\mathbf{f}(\mathbf{x},t)$ is generated by the elastic and approximately inextensible rotating flagellum, which rotates with period T. We model $\mathbf{f}(\mathbf{x},t)$ using the immersed boundary method, whereby forces and torques generated by the flagellum are spread out into the fluid by convolving one-dimensional Lagrangian force and torque densities against regularized delta functions. The resulting Eulerian force density $\mathbf{f}(\mathbf{x},t)$ is given by

$$\mathbf{f}(\mathbf{x},t) = \int_0^{\ell} \frac{\partial \mathbf{F}^{\mathrm{rod}}(s,t)}{\partial s} \delta_w(\mathbf{x} - \chi(s,t))\,\mathrm{d}s + \frac{1}{2}\nabla \times \int_0^{\ell} \left(\frac{\partial \mathbf{N}^{\mathrm{rod}}(s,t)}{\partial s} + \left(\frac{\partial \chi(s,t)}{\partial s} \times \mathbf{F}^{\mathrm{rod}} \right) \right) \delta_w(\mathbf{x} - \chi(s,t))\,\mathrm{d}s, \tag{4}$$

in which $\chi(s,t)$ is physical location of the centerline of the flagellum at time t and ℓ is the length of the flagellum in the reference configuration. We delay defining $\mathbf{F}^{\mathrm{rod}}(s,t)$ and $\mathbf{N}^{\mathrm{rod}}(s,t)$ until later because we will first seek to non-dimensionalize the Eulerian equations of motion, and then subsequently the Lagrangian equations which model the elasticity and inextensibility of the flagellum.

To non-dimensionalize this system of equations, we start by noting that the conformation tensor $\mathbb{C}(\mathbf{x},t)$ is already dimensionless. We choose to non-dimensionalize space, time, velocity, and pressure using the following rescalings

- $t \longrightarrow Tt$,
- $\mathbf{x} \longrightarrow L\mathbf{x}$,
- $\mathbf{u} \longrightarrow \frac{L}{T}\mathbf{u}$,
- $p \longrightarrow \frac{\mu}{T}p$,

in which $\mu = \mu_\text{n} + \mu_\text{p}$ is the total viscosity of the fluid and L is a characteristic length scale. After applying the chain rule and performing some algebraic manipulations, equation (1) may be rewritten as

$$\frac{\rho L^2}{T\mu}\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} = \frac{\mu_\text{n}}{\mu}\Delta \mathbf{u}(\mathbf{x},t) - \nabla p + \frac{\mu_\text{p} T}{\mu \lambda}\nabla \cdot \mathbb{C}(\mathbf{x},t) + \frac{LT}{\mu}\mathbf{f}(\mathbf{x},t). \tag{5}$$

We next identify dimensionless parameters: the Reynolds number Re, the Deborah number De, and the ratio of polymeric viscosity to the total viscosity β. These are given by

- $\text{Re} = \frac{\rho L^2}{T\mu}$
- $\text{De} = \frac{\lambda}{T}$
- $\beta = \frac{\mu_\text{p}}{\mu}$

After making these identifications, the dimensionless formulation of the fluid momentum equation is

$$\text{Re}\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} = (1-\beta)\Delta \mathbf{u}(\mathbf{x},t) - \nabla p(\mathbf{x},t) + \frac{\beta}{\text{De}}\nabla \cdot \mathbb{C}(\mathbf{x},t) + \frac{LT}{\mu}\mathbf{f}(\mathbf{x},t). \tag{6}$$

The time, space, and velocity rescalings yield the following dimensionless formulation of the Giesekus equation

$$\text{De}\ \overset{\triangledown}{\mathbb{C}}(\mathbf{x},t) = -(\mathbb{C}(\mathbf{x},t) - \mathbb{I}) - \alpha(\mathbb{C}(\mathbf{x},t) - \mathbb{I})^2. \tag{7}$$

Next, we consider the non-dimensionalization of the Eulerian force density $\mathbf{f}(\mathbf{x},t)$. Isolating $\frac{LT}{\mu}\mathbf{f}(\mathbf{x},t)$ in equation (6), we have

$$\frac{LT}{\mu}\mathbf{f}(\mathbf{x},t) = \frac{LT}{\mu}\int_0^\ell \frac{\partial \mathbf{F}^\text{rod}}{\partial s}\delta_w\left(L\mathbf{x} - \boldsymbol{\chi}(s,t)\right)\,\mathrm{d}s + \frac{T}{\mu}\nabla \times \int_0^\ell \left(\frac{\partial \mathbf{N}(s,t)}{\partial s} + \frac{\partial \boldsymbol{\chi}(s,t)}{\partial s} \times \mathbf{F}^\text{rod}\right)\delta_w\left(L\mathbf{x} - \boldsymbol{\chi}(s,t)\right)\,\mathrm{d}s, \tag{8}$$

in which ℓ is the length of the flagellum. If we rescale the Lagrangian reference coordinate to $s \longrightarrow Ls$, the physical location of the centerline to $\boldsymbol{\chi}(s,t) \longrightarrow L\boldsymbol{\chi}(Ls,t)$, and the width of the regularized delta function to $w \longrightarrow Lw$, then the right hand side of equation (8) becomes

$$\frac{T}{\mu L^2}\int_0^{\ell/L} \frac{\partial \mathbf{F}^\text{rod}(s,t)}{\partial s}\delta_w\left(\mathbf{x} - \boldsymbol{\chi}(s,t)\right)\,\mathrm{d}s + \frac{T}{2\mu L^3}\nabla \times \int_0^{\ell/L}\left(\frac{\partial \mathbf{N}^\text{rod}(\mathbf{x},t)}{\partial s}\right)\delta_w\left(\mathbf{x} - \boldsymbol{\chi}(s,t)\right)\,\mathrm{d}s \tag{9}$$

$$+ \frac{T}{2\mu L^2}\nabla \times \int_0^{\ell/L}\left(\frac{\partial \boldsymbol{\chi}(s,t)}{\partial s} \times \mathbf{F}^\text{rod}(s,t)\right)\delta_w(\mathbf{x} - \boldsymbol{\chi}(s,t))\,\mathrm{d}s \tag{10}$$

To continue converting the equations into a dimensionless formulation, we next rescale the Lagrangian force $\mathbf{F}^\text{rod}$ and torque $\mathbf{N}^\text{rod}$. To do this, we will need their definitions. Because we are using Kirchhoff rod theory to model, the Lagrangian forces and torques are projected onto the set of unit (and dimensionless) director vectors $\{\mathbb{D}_i(s,t)\}_{i=1}^3$

$$\mathbf{F}^\text{rod}(s,t) = \sum_{i=1}^3 F_i^\text{rod}\mathbb{D}_i(s,t), \quad \text{and} \quad \mathbf{N}^\text{rod}(s,t) = \sum_{i=1}^3 N_i^\text{rod}\mathbb{D}_i(s,t).$$

The coefficients of each vector represented in this basis are given by

$$F_i^\text{rod} = b_i\left(\frac{\partial \boldsymbol{\chi}(s,t)}{\partial s}\cdot \mathbb{D}_i(s,t) - \delta_{3,i}\right), \quad i = 1,2,3, \tag{11}$$

$$N_1^\text{rod} = a_1\left(\Omega_1(s,t) - \kappa_1\right), \tag{12}$$

$$N_2^\text{rod} = a_2\left(\Omega_2(s,t) - \kappa_2\right), \tag{13}$$

$$N_3^\text{rod} = a_3\left(\Omega_3(s,t) - \tau_1\right)\left(\Omega_3(s,t) - \tau_2\right)\left(\Omega_3(s,t) - \frac{\tau_1+\tau_2}{2}\right) - \frac{\gamma^2}{L^2}\frac{\partial^2 \Omega_3(s,t)}{\partial s^2}. \tag{14}$$

To nondimensionalize these forces and torques, we first nondimensionalize the Ω_1, Ω_2, and Ω_3 vectors, which have units of inverse length. We rescale Ω_1 and Ω_2 according to:

- $\Omega_1 \longrightarrow \kappa_1 \Omega_1$
- $\Omega_2 \longrightarrow \kappa_2 \Omega_2$

The choice of rescaling for Ω_3 is less obvious because there are multiple parameters that define the third component of the torque N_3^{rod}. Assuming $\tau_1 = -\tau_2$ so that the flagellum has equal but opposite intrinsic twists, the equation for N_3^{rod} becomes

$$N_3^{\text{rod}} = a_3\left(\Omega_3(s,t) + \tau\right)\left(\Omega_3(s,t) - \tau\right)\Omega_3(s,t) - \frac{\gamma^2}{L^2}\frac{\partial^2 \Omega_3(s,t)}{\partial s^2}, \tag{15}$$

in which $\tau = -\tau_1 = \tau_2$. Therefore, we decide to rescale Ω_3 according to $\Omega_3 \rightarrow \tau\Omega_3$. After applying these rescalings, we choose to rescale the Lagrangian forces and torques by their respective coefficients.

- $F_1^{\text{rod}} \longrightarrow b_1 F_1^{\text{rod}}$
- $F_2^{\text{rod}} \longrightarrow b_2 F_2^{\text{rod}}$
- $F_3^{\text{rod}} \longrightarrow b_3 F_3^{\text{rod}}$
- $N_1^{\text{rod}} \longrightarrow a_1 \kappa_1 N_1^{\text{rod}}$
- $N_2^{\text{rod}} \longrightarrow a_2 \kappa_2 N_2^{\text{rod}}$
- $N_3^{\text{rod}} \longrightarrow a_3 \tau^3 N_3^{\text{rod}}$

Using these rescalings, the dimensionless Eulerian force density $\frac{LT}{\mu_s}\mathbf{f}(\mathbf{x},t)$ takes the form

$$\begin{aligned}
\frac{LT}{\mu}\mathbf{f}(\mathbf{x},t) = {} & \frac{T}{\mu L^2}\int_0^{\ell/L}\sum_{i=1}^{3}\frac{\partial}{\partial s}\left(b_i F_i^{\text{rod}}\mathbb{D}_i(s,t)\right)\delta_w\left(\mathbf{x}-\boldsymbol{\chi}(s,t)\right)\,\mathrm{d}s \\
& + \nabla\times\frac{T}{2\mu L^3}\int_0^{\ell/L}\left(\kappa_1 a_1\frac{\partial}{\partial s}N_1^{\text{rod}}\mathbb{D}_1(s,t) + \kappa_2 a_2\frac{\partial}{\partial s}N_2^{\text{rod}}\mathbb{D}_2(s,t) + a_3\tau^3\frac{\partial}{\partial s}N_3^{\text{rod}}\mathbb{D}_3(s,t)\right)\delta_w\left(\mathbf{x}-\boldsymbol{\chi}(s,t)\right)\,\mathrm{d}s \\
& + \nabla\times\frac{T}{2\mu L^2}\int_0^{\ell/L}\left(\frac{\partial\boldsymbol{\chi}(s,t)}{\partial s}\times\sum_{i=1}^{3}b_i F_i^{\text{rod}}\mathbb{D}_i(s,t)\right)\delta_w\left(\mathbf{x}-\boldsymbol{\chi}(s,t)\right)\,\mathrm{d}s.
\end{aligned} \tag{16}$$

This dimensionless Eulerian force density enables us to identify several important dimensionless timescales. The dimensionless timescales associated with the stretching forces take the form

$$\frac{T}{\mu_s L^2 b_i^{-1}} \text{ for } i = 1, 2, 3. \tag{17}$$

The dimensionless timescales associated with the bending motion of the flagellum are

$$\frac{T}{2\mu_s L^3(\kappa_1 a_1)^{-1}} \quad \text{and} \quad \frac{T}{2\mu_s L^3(\kappa_2 a_2)^{-1}}. \tag{18}$$

The dimensionless timescales associated with the twisting motion of the flagellum is

$$\frac{T}{2\mu_s L^3\left(\tau^3 a_3\right)^{-1}}. \tag{19}$$

These dimensionless timescales represent the ratio of the period of the flagellar motor rotation to the characteristic stretching, bending, and twisting motions of the flagella's filament. Note that these nondimensionless scalings assume κ_1 and κ_2 are constant along the length of the flagellum's filament. If κ_1 and κ_2 are non-constant, we may choose to rescale Ω_1 and Ω_2 as $\Omega_1 \rightarrow \frac{1}{L}\Omega_1$ and $\Omega_2 \rightarrow \frac{1}{L}\Omega_2$.

For the parameters used in this study, we find the following dimensional time scales

$$T^{\mathrm{stretch}} = \mu L^2 b^{-1} \approx 2 \times 10^{-7}\,\mathrm{s}, \tag{20}$$

$$T^{\mathrm{bend}} = 2\mu L^3 (\kappa a)^{-1} \approx 3 \times 10^{-5}\,\mathrm{s}, \tag{21}$$

$$T^{\mathrm{twist}} = 2\mu L^3 \left(\tau^3 a_3\right)^{-1} \approx 1 \times 10^{-4}\,\mathrm{s}, \tag{22}$$

in which we have chosen the length scale to be the initial radius of the flagellum, $L = R_0$. When compared with the rotation period of the motor, $T_s = 0.01$ s, we find that the timescales of the flagellum are much shorter than that of the motor, effectively making the flagellum a 'stiff body'.[2] The relaxation times of the fluid used in the following results vary between $\lambda = 1 \times 10^{-4}$ s to 2×10^{-2} s, making the timescales of stretching and bending much shorter than the elastic relaxation time of the fluid. The twisting timescale, however, can be on the same order as the relaxation time of the fluid.

REFERENCES

[1] S. A. Khan and R. G. Larson. Comparison of Simple Constitutive Equations for Polymer Melts in Shear and Biaxial and Uniaxial Extensions. *Journal of Rheology*, 31(3):207–234, 04 1987.

[2] Becca Thomases and Robert D. Guy. The role of body flexibility in stroke enhancements for finite-length undulatory swimmers in viscoelastic fluids. *Journal of Fluid Mechanics*, 825:109–132, 2017.